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Two New Sesquiterpenes from *Inula japonica*

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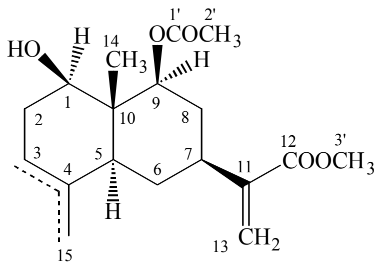
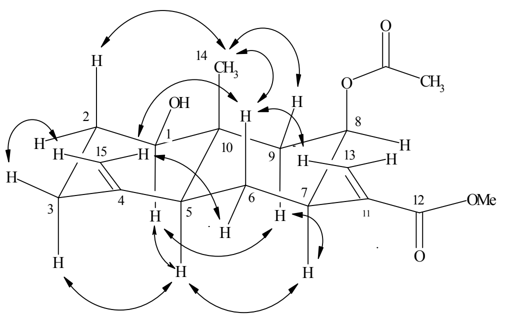
Abstract: Two new sesquiterpenes were isolated from the aerial parts of *Inula japonica*. Their structures were elucidated as 1β-hydroxy-8β-acetoxycostic acid methyl ester and 1β-hydroxy-8β-acetoxyisocostic acid methyl ester by spectral methods.

Keywords: *Inula Japonica*, Compositae, sesquiterpene.

The research of the aerial parts of *Inula japonica* Thunb, a Chinese folk medicine for antitussive and antidropsical properties[1] led to the isolation of two new sesquiterpenes **1** and **2**. Here we report the structure elucidation of them.

Figure 1 Key NOE correlation of compound **1**





1 Δ 4(15)
2 Δ 3

Compound **1**, $C_{18}H_{26}O_5$ (HRMS: *m/z* = 323.1858 $[M+H]^+$, calcd. 322.1853), was isolated as colorless oil. Its IR spectrum exhibited strong absorptions at 3424, 1729, 1712, 1650, 1625, 1242 cm^{-1}. The structure of compound **1** followed from its ^1H NMR and ^{13}C NMR (DEPT) data (**Table 1**) which were in part close to those of 8β-acetoxycostic acid methyl ester[2]. An additional hydroxy group was required for the molecular formula $C_{18}H_{26}O_5$, and the signals appeared at δ_H 3.43 (dd, 1H, *J*= 11.5, 5.0Hz) and δ_C 79.2 (CH) suggested the hydroxy group was at C-1. The coupling of H-1 ($J_{1, 2\beta}$=

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11.5Hz) indicated a 1β-hydroxy group. The ^{1}H-^{13}C long-range correlations (**Table 1**) in HMBC experiment and the correlation points (shown by arrows in **Figure 1**) in ^{1}H-^{1}H NOESY spectra further confirmed the above structural elucidation of **1**. Consequently, compound **1** was characterized as 1β-hydroxy-8β-acetoxycostic acid methyl ester.

Compound **2** was obtained as colorless oil, also had the molecular formula $C_{18}H_{26}O_5$ (EIMS: $m/z = 322$ $[M]^+$). Its ^{1}H and ^{13}C NMR spectra (**Table 1**) clearly showed that **2** was a Δ^3-isomer of compound **1**. So the structure of **2** was determined as 1β-hydroxy-8β-acetoxyisocostic acid methyl ester.

Table 1 ^{1}H, ^{13}C NMR (DEPT) and HMBC data of **1** and **2** ($CDCl_3$, TMS, δ, ppm)

NO.	^{1}H (α / β) **1**	^{13}C **1**	HMBC(C/H) **1**	^{1}H (α / β) **2**	^{13}C **2**
1	3.43 (dd, 12.0, 5.0)	79.2 d	C-1 / H-3, 5, 9, 14	3.57 (dd, 10.0, 7.0)	76.7 d
2	1.79 (brddd, 13.0, 5.0, 5.0) 1.60 (dddd, 13, 12, 12, 5.0)	30.8 t	C-2 / H-1, 3	2.34 (ddd, 14, 7, 3) 1.93 (ddd, 14, 10, 3)	32.3 t
3	2.12 (brddd,13.8, 12.0, 5.0) 2.32 (ddd, 13.8, 5.0, 3.0)	33.8 t	C-3 / H-1, 5, 15	5.31 (dd, 3, 3)	120.0 d
4	-	147.8 s	C-4 / H-2, 6, 15	-	134.2 s
5	1.91(dd, 12.5, 4.0)	47.6 d	C-5 / H-1, 3, 9, 14, 15	2.02 (brd, 11)	46.5 d
6	1.48 (ddd, 14.0, 4.0, 2.0) 1.86 (ddd, 14.0, 12.5, 11.5)	23.2 t	C-6 / H-5, 7, 8	1.66-1.56* (m)	23.2 t
7	2.89 (brd, 11.5)	41.5 d	C-7 / H-6, 9, 13	2.88 (m, 8, 7, 3)	42.5 d
8	5.29 (brs)	69.5 d	C-8 / H-6, 9	5.31 (brdd, 3.5, 3)	69.3 d
9	1.52 (dd, 15.0, 2.5) 2.25 (dd, 15.0, 2.2)	40.6 t	C-9 / H-5, 14	1.46 (dd, 14.5, 3.5) 1.80 (brd, 14.5)	39.3 t
10	-	39.9 s	C-10 / H-1, 2, 6, 8, 14	-	37.2 s
11	-	140.9 s	C-11 / H-6, 7, 13	-	140.9 s
12	-	167.0 s	C-12 / H-3′, 11, 13	-	167.1 s
13	6.27 (d, 1.5) 5.62 (d, 1.5)	125.2 t	-	6.28 (br.s) 5.60 (br.s)	125.4 t
14	0.84 (s)	12.0 q	C-14 / H-1, 5, 9	0.95 (s)	11.0 q
15	4.80 (br.s) 4.59 (br.s)	106.9 t	C-15 / H-3, 5	1.65 (br.s)	20.8 t
1′	-	170.1 s	C-1′ / H-2′, 8	-	170.2 s
2′	1.94 (s)	21.1 q	-	1.96 (s)	21.2 q
3′	3.75 (s)	52.0 q	-	3.76 (s)	52.0 q

Acknowledgment

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References

1. Jiangsu New Medical College, *A Dictionary of Traditional Chinese Drugs*, Shanghai People's Press, Shanghai, **1977**, p.324.
2. C. Zdero, F. Bohlmann, *Phytochemistry*, **1989**, *28* (11), 3105.

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